Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.15e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.42e-01

Confidence level: 3.03e-01

Nearest Neighbors from the Training Set

Image not found
2-Ethylhexyl diphenyl phosphate
Measured: 3.00e-10
Predicted: 1.52e-05

Image not found
Isophorone diamine
Measured: 4.00e-14
Predicted: 1.87e-02

Image not found
Tetrachlorovinphos
Measured: 3.00e-09
Predicted: 9.39e-07

Image not found
Z-Tetrachlorvinphos
Measured: 3.00e-09
Predicted: 9.39e-07

Image not found
Halfenprox
Measured: 1.35e-06
Predicted: 7.31e-09

Image not found
Fludioxonil
Measured: 1.35e-07
Predicted: 1.63e-08